

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
 Data File : VV037336.D  
 Acq On : 18 Sep 2024 16:09  
 Operator : SY/MD  
 Sample : P3988-09  
 Misc : 25mL/MSVOA\_V/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BH8R8

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV037336.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.101       | 11            | 19          | 47           | rVB      | 74644          | 193084        | 2.54%           | 0.784%        |
| 2         | 1.281       | 65            | 75          | 83           | rBV2     | 627540         | 693433        | 9.13%           | 2.816%        |
| 3         | 1.333       | 83            | 91          | 115          | rVV      | 160893         | 547373        | 7.21%           | 2.223%        |
| 4         | 1.433       | 116           | 122         | 135          | rVV      | 113221         | 172385        | 2.27%           | 0.700%        |
| 5         | 1.529       | 147           | 152         | 168          | rVB      | 120210         | 163815        | 2.16%           | 0.665%        |
| 6         | 1.982       | 286           | 293         | 306          | rVV      | 89898          | 140542        | 1.85%           | 0.571%        |
| 7         | 2.066       | 307           | 319         | 332          | rVV      | 1777366        | 2707856       | 35.66%          | 10.995%       |
| 8         | 2.133       | 332           | 340         | 365          | rVB2     | 114794         | 307594        | 4.05%           | 1.249%        |
| 9         | 3.104       | 627           | 642         | 668          | rBV      | 662129         | 1393899       | 18.36%          | 5.660%        |
| 10        | 3.584       | 775           | 791         | 815          | rBV      | 163374         | 431602        | 5.68%           | 1.752%        |
| 11        | 3.802       | 845           | 859         | 877          | rBV      | 3178335        | 7594047       | 100.00%         | 30.835%       |
| 12        | 4.243       | 982           | 996         | 1035         | rBV      | 157841         | 439270        | 5.78%           | 1.784%        |
| 13        | 4.953       | 1202          | 1217        | 1247         | rBV2     | 367723         | 970540        | 12.78%          | 3.941%        |
| 14        | 5.532       | 1387          | 1397        | 1431         | rBV      | 278817         | 611133        | 8.05%           | 2.481%        |
| 15        | 5.825       | 1476          | 1488        | 1524         | rBV      | 1345191        | 2727433       | 35.92%          | 11.075%       |
| 16        | 5.985       | 1527          | 1538        | 1561         | rVV2     | 212396         | 462944        | 6.10%           | 1.880%        |
| 17        | 6.915       | 1816          | 1827        | 1848         | rBV      | 85961          | 187463        | 2.47%           | 0.761%        |
| 18        | 7.239       | 1918          | 1928        | 1948         | rBV      | 408201         | 763168        | 10.05%          | 3.099%        |
| 19        | 7.558       | 2017          | 2027        | 2044         | rBV      | 47305          | 99576         | 1.31%           | 0.404%        |
| 20        | 8.024       | 2163          | 2172        | 2208         | rBV      | 458191         | 1043767       | 13.74%          | 4.238%        |
| 21        | 8.779       | 2397          | 2407        | 2434         | rBV      | 465692         | 831845        | 10.95%          | 3.378%        |
| 22        | 10.149      | 2822          | 2833        | 2856         | rVB      | 182050         | 303322        | 3.99%           | 1.232%        |
| 23        | 11.181      | 3145          | 3154        | 3180         | rVB      | 490688         | 811131        | 10.68%          | 3.294%        |
| 24        | 11.484      | 3238          | 3248        | 3261         | rBV2     | 108679         | 221642        | 2.92%           | 0.900%        |
| 25        | 11.554      | 3261          | 3270        | 3299         | rVB      | 467981         | 809016        | 10.65%          | 3.285%        |

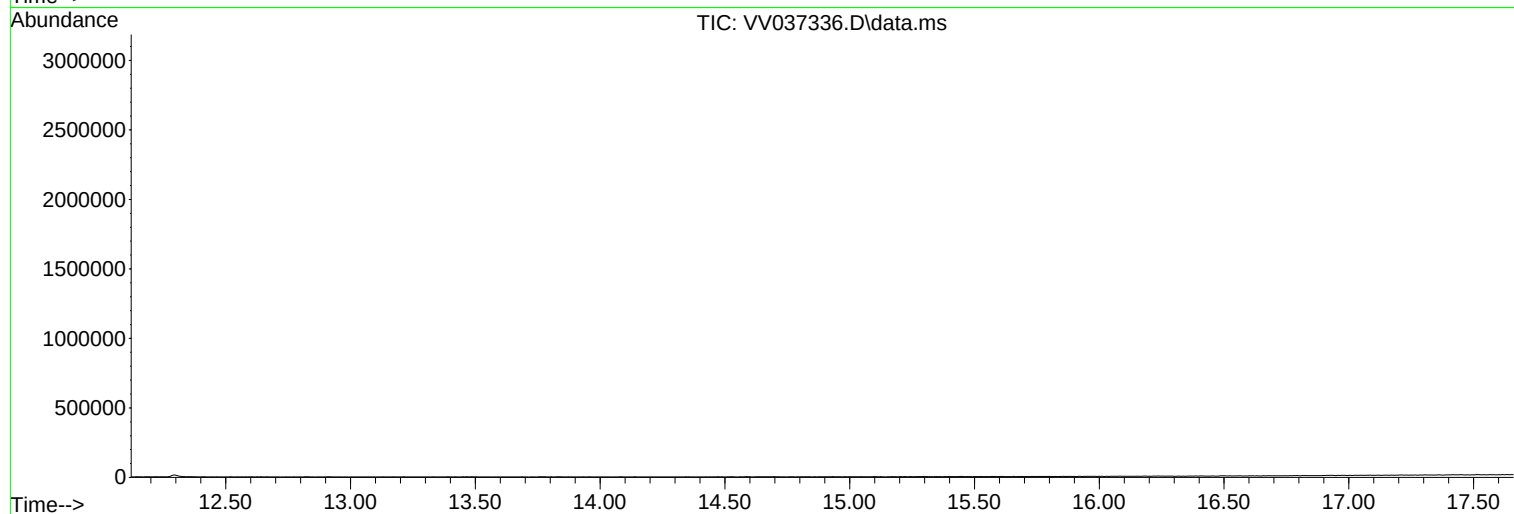
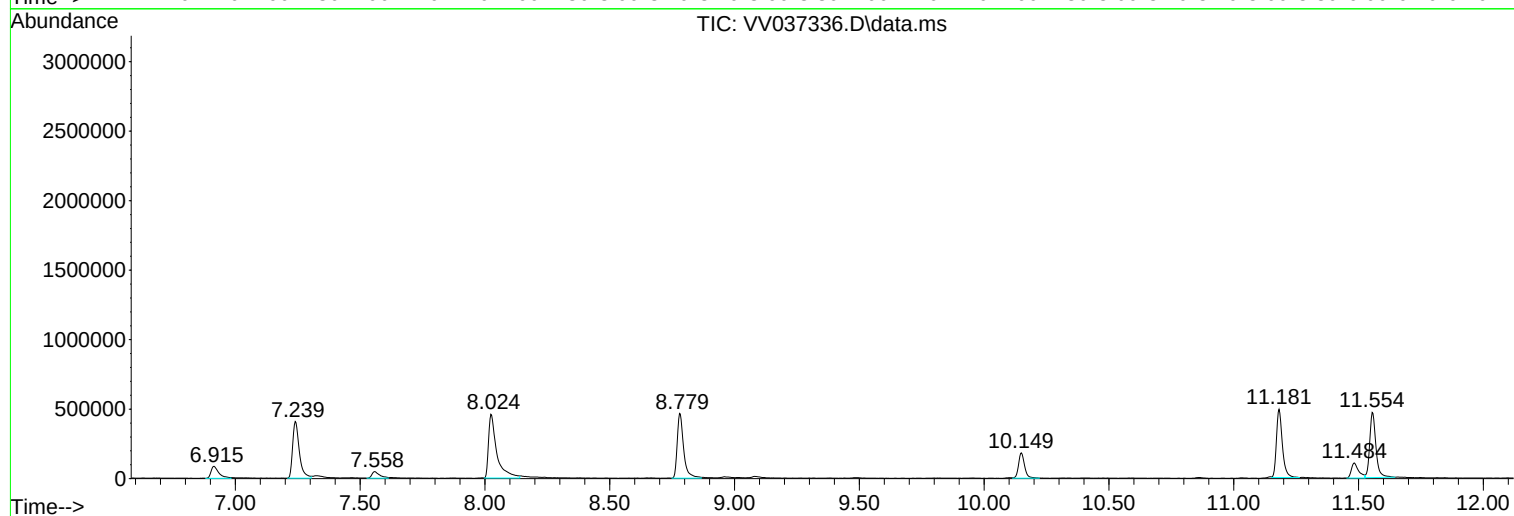
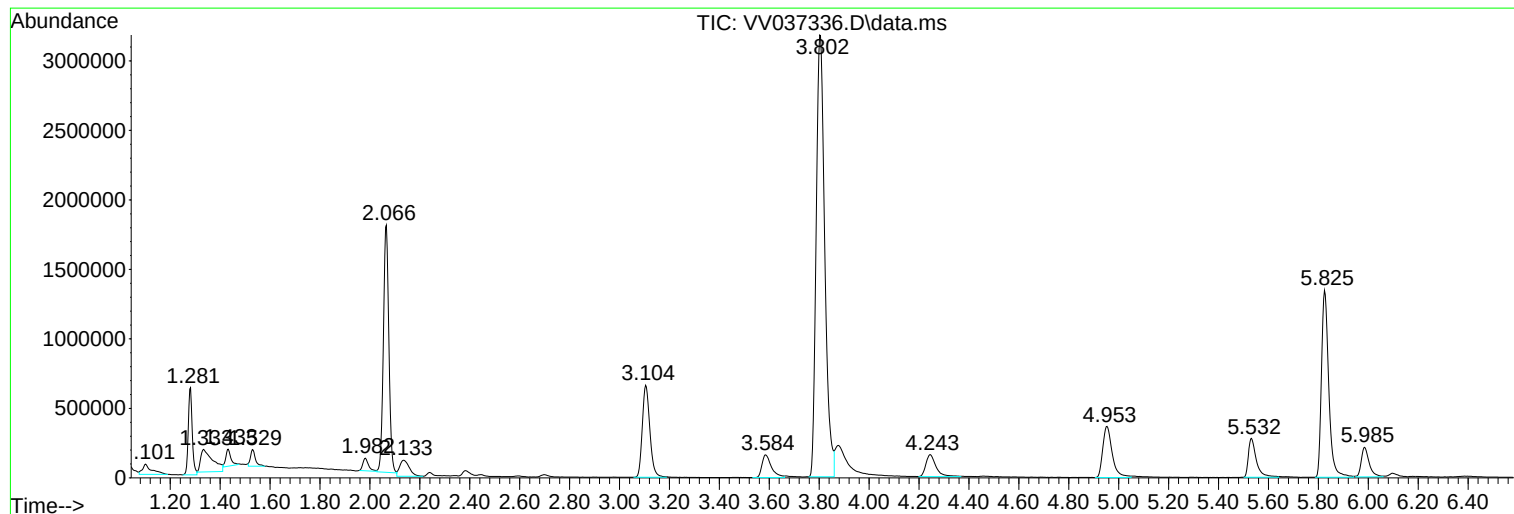
Sum of corrected areas: 24627880

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

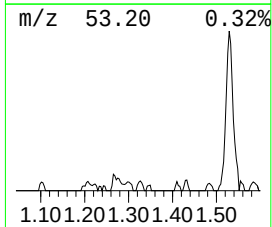
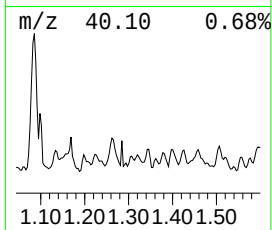
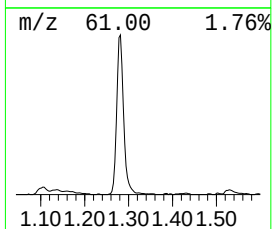
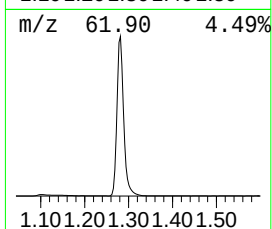
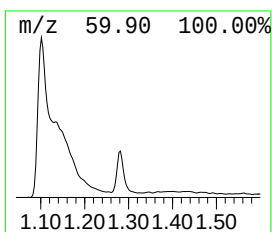
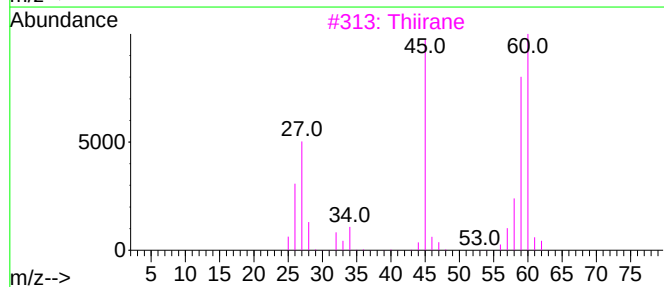
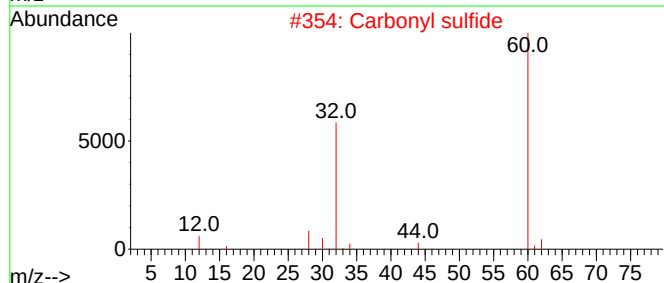
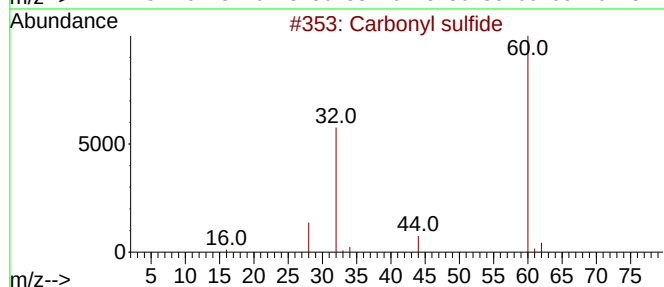
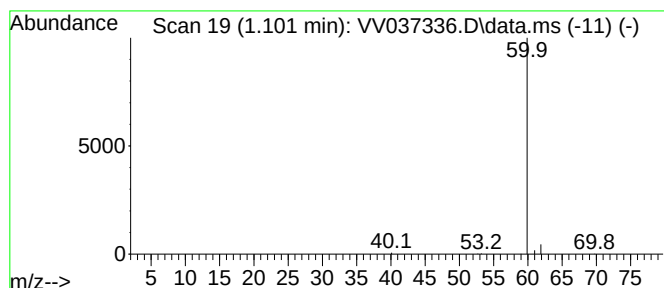
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 unknown-01 Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.101 | 1.58 ug/L | 193084 | 1,4-Difluorobenzene | 5.532 |

| Hit# | of | 5 | Tentative ID     | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------|----|---------|-------------|------|
| 1    |    |   | Carbonyl sulfide | 60 | COS     | 000463-58-1 | 5    |
| 2    |    |   | Carbonyl sulfide | 60 | COS     | 000463-58-1 | 5    |
| 3    |    |   | Thiirane         | 60 | C2H4S   | 000420-12-2 | 4    |
| 4    |    |   | Formamidoxime    | 60 | CH4N2O  | 000624-82-8 | 4    |
| 5    |    |   | Urea             | 60 | CH4N2O  | 000057-13-6 | 4    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

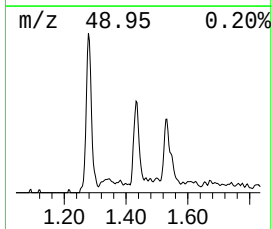
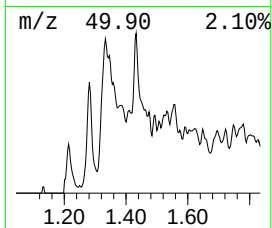
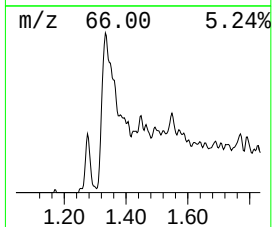
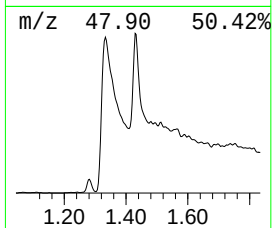
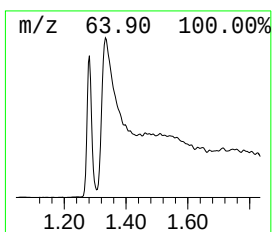
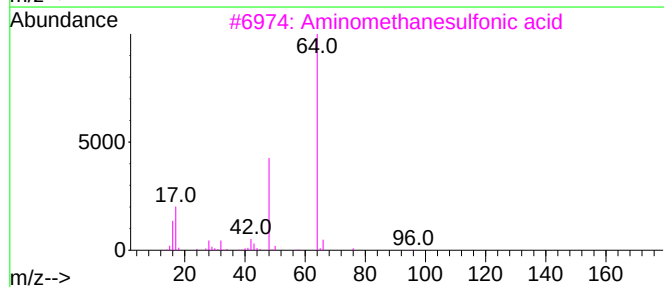
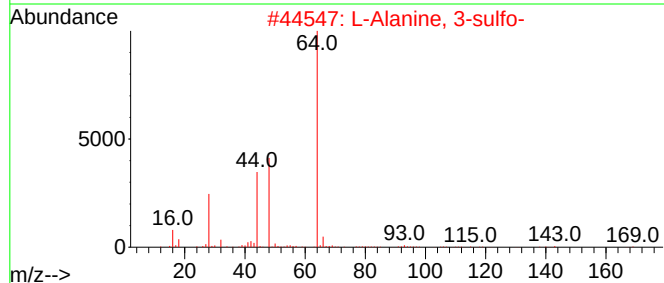
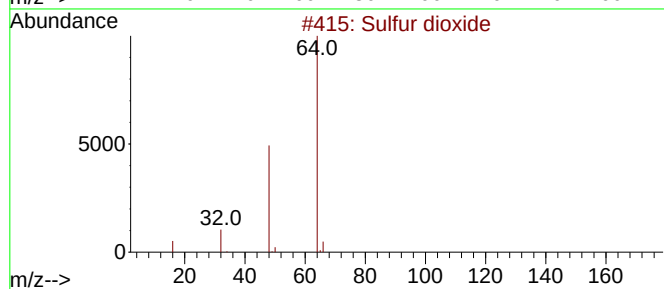
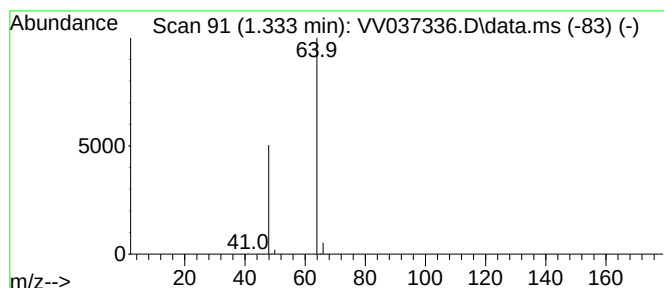
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.333 | 4.48 ug/L | 547373 | 1,4-Difluorobenzene | 5.532 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 74   |
| 2    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 3    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 4    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 4    |
| 5    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

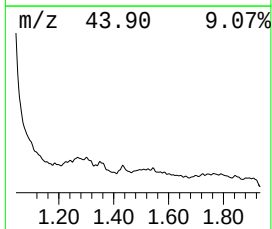
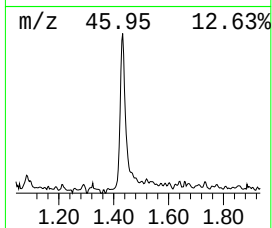
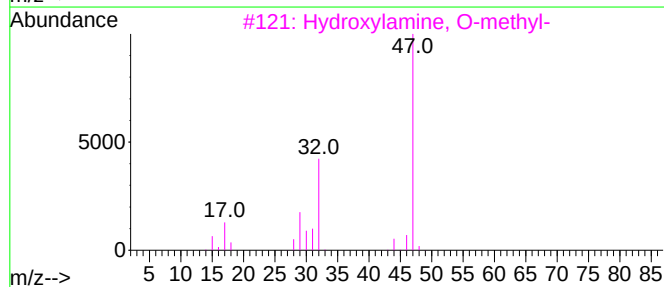
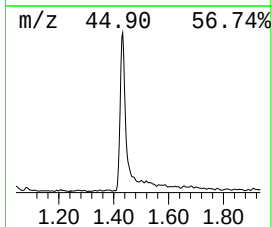
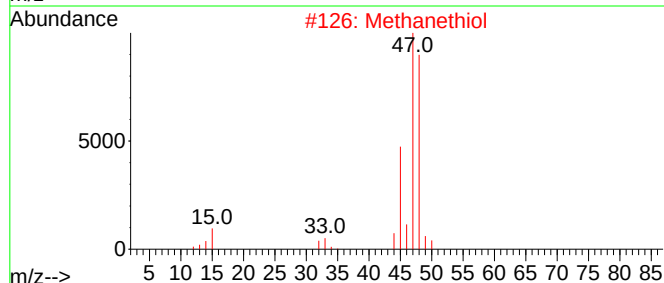
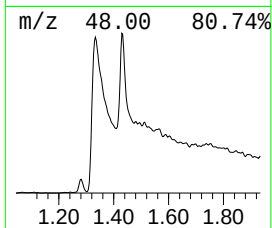
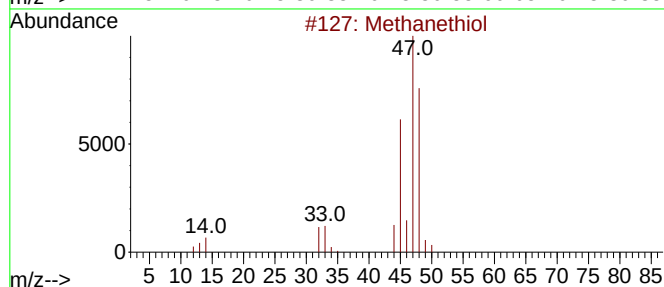
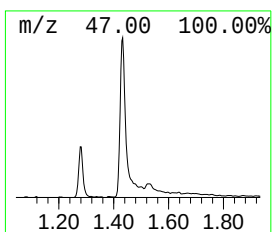
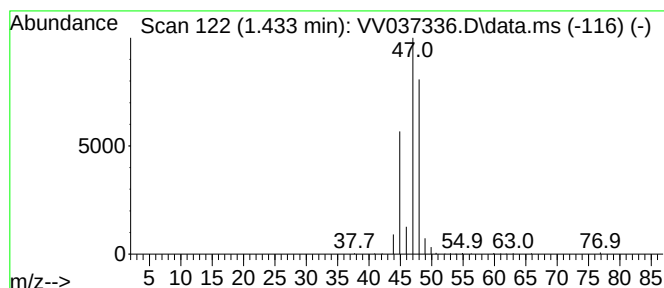
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Methanethiol Concentration Rank 5

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.433 | 1.41 ug/L | 172385 | 1,4-Difluorobenzene | 5.532 |

| Hit# | of | 5 | Tentative ID             | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|----|---------|-------------|------|
| 1    |    |   | Methanethiol             | 48 | CH4S    | 000074-93-1 | 91   |
| 2    |    |   | Methanethiol             | 48 | CH4S    | 000074-93-1 | 90   |
| 3    |    |   | Hydroxylamine, O-methyl- | 47 | CH5NO   | 000067-62-9 | 7    |
| 4    |    |   | Hydroxylamine, O-methyl- | 47 | CH5NO   | 000067-62-9 | 7    |
| 5    |    |   | Methane, nitroso-        | 45 | CH3NO   | 000865-40-7 | 5    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

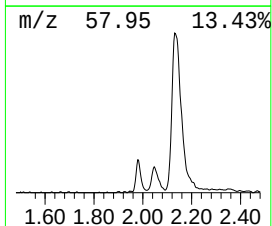
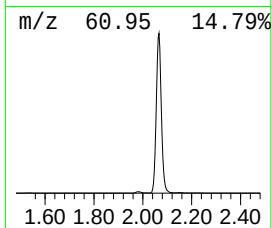
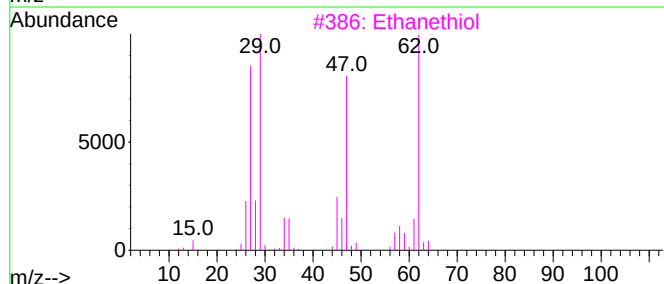
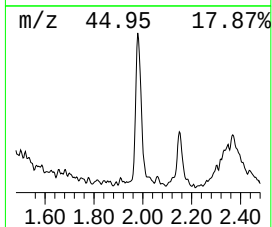
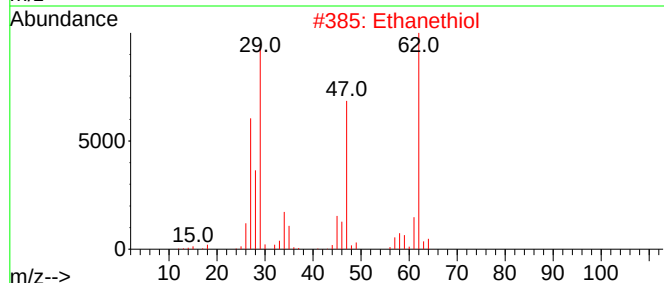
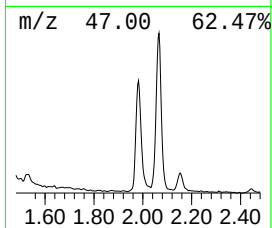
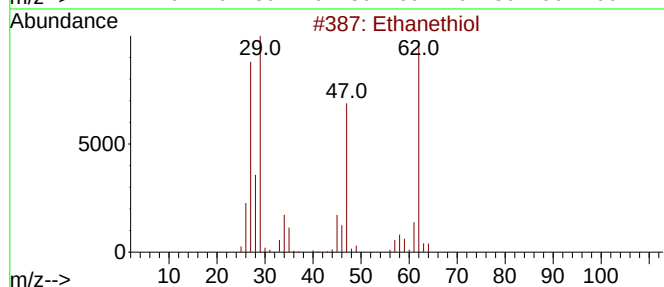
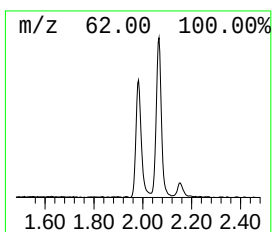
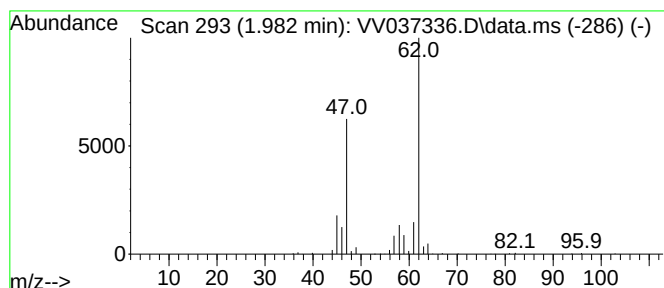
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 4 Ethanethiol Concentration Rank 7

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.982 | 1.15 ug/L | 140542 | 1,4-Difluorobenzene | 5.532 |

| Hit# | of          | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|-------------|---|--------------|----|---------|-------------|------|
| 1    | Ethanethiol |   |              | 62 | C2H6S   | 000075-08-1 | 91   |
| 2    | Ethanethiol |   |              | 62 | C2H6S   | 000075-08-1 | 91   |
| 3    | Ethanethiol |   |              | 62 | C2H6S   | 000075-08-1 | 91   |
| 4    | Ethanethiol |   |              | 62 | C2H6S   | 000075-08-1 | 91   |
| 5    | Ethanethiol |   |              | 62 | C2H6S   | 000075-08-1 | 87   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

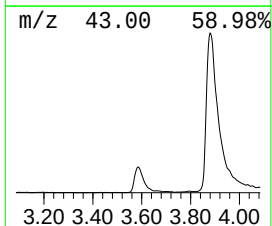
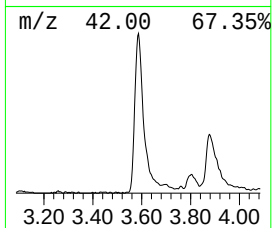
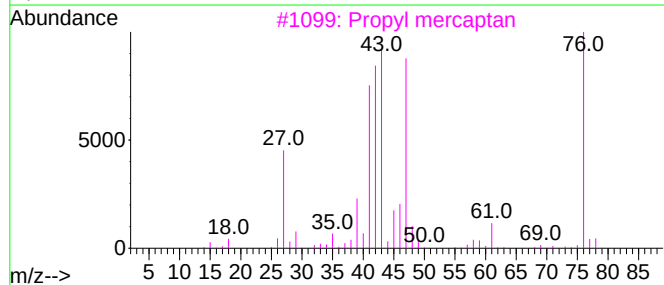
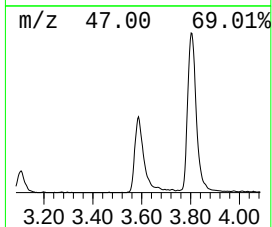
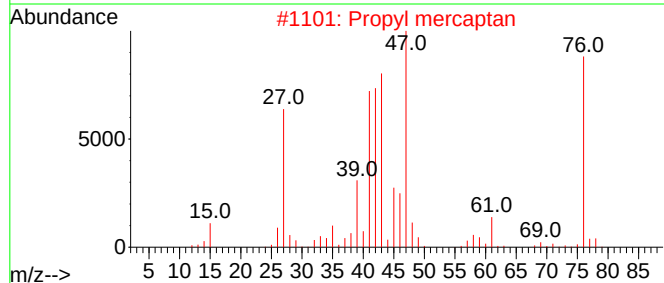
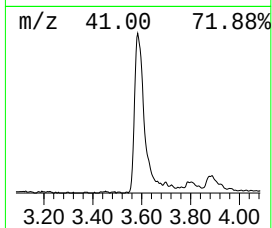
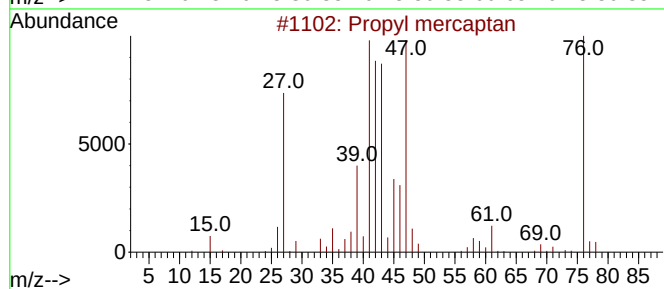
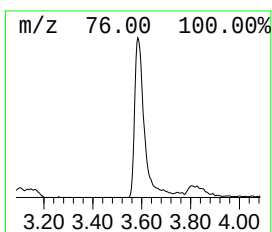
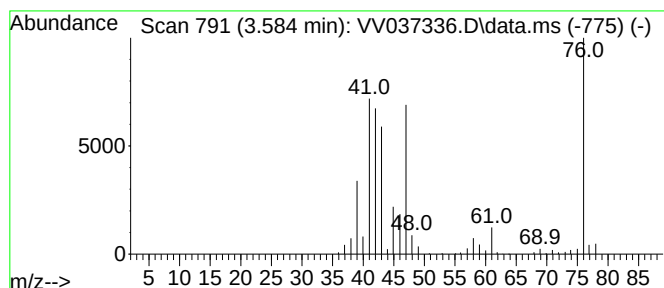
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Propyl mercaptan Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 3.584 | 3.53 ug/L | 431602 | 1,4-Difluorobenzene | 5.532 |

| Hit# | of               | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|------------------|---|--------------|----|---------|-------------|------|
| 1    | Propyl mercaptan |   |              | 76 | C3H8S   | 000107-03-9 | 91   |
| 2    | Propyl mercaptan |   |              | 76 | C3H8S   | 000107-03-9 | 91   |
| 3    | Propyl mercaptan |   |              | 76 | C3H8S   | 000107-03-9 | 91   |
| 4    | Propyl mercaptan |   |              | 76 | C3H8S   | 000107-03-9 | 91   |
| 5    | Propyl mercaptan |   |              | 76 | C3H8S   | 000107-03-9 | 91   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

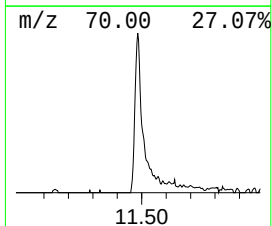
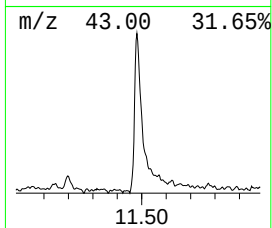
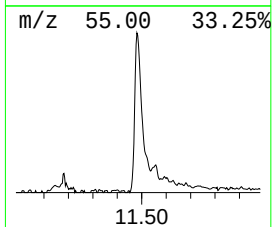
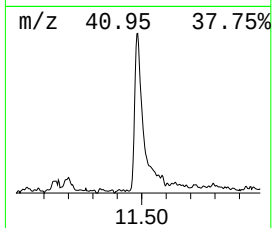
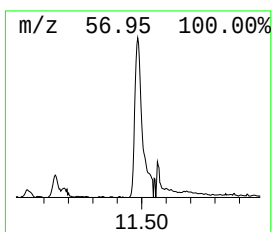
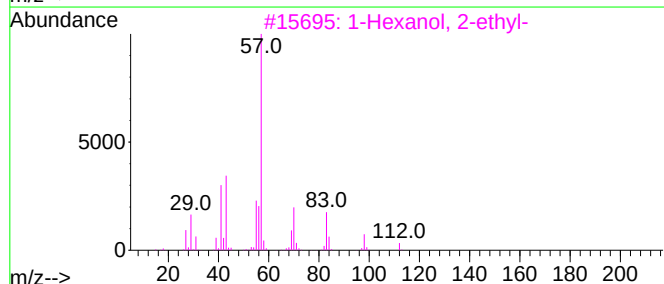
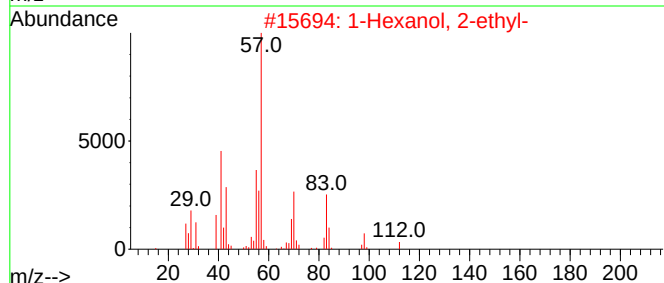
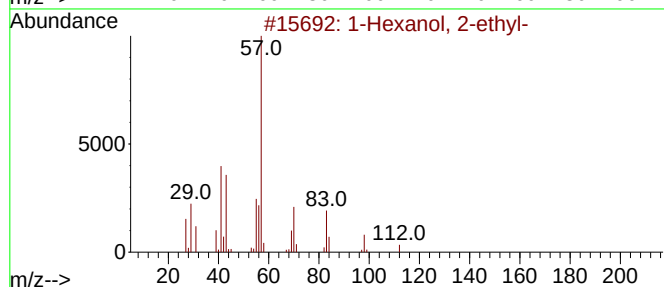
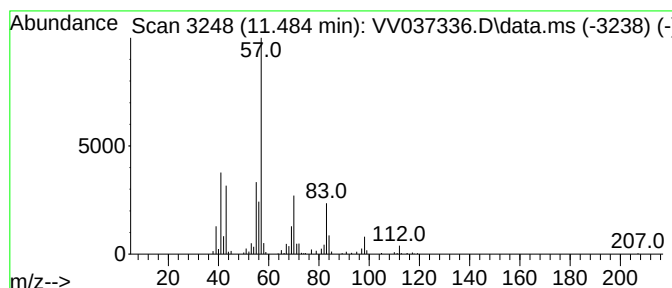
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 6

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 11.484 | 1.37 ug/L | 221642 | 1,4-Dichlorobenzene-d4 | 11.181 |

| Hit# | of                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 3    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 4    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 83   |
| 5    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 78   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\DATA\VV091824\  
Data File : VV037336.D  
Acq On : 18 Sep 2024 16:09  
Operator : SY/MD  
Sample : P3988-09  
Misc : 25mL/MSVOA\_V/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BH8R8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR091024WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| unknown-01         | 1.101  | 1.6     | ug/L  | 193084   | 1                     | 5.532  | 611133 | 5.0  |
| Sulfur dioxide     | 1.333  | 4.5     | ug/L  | 547373   | 1                     | 5.532  | 611133 | 5.0  |
| Methanethiol       | 1.433  | 1.4     | ug/L  | 172385   | 1                     | 5.532  | 611133 | 5.0  |
| Ethanethiol        | 1.982  | 1.1     | ug/L  | 140542   | 1                     | 5.532  | 611133 | 5.0  |
| Propyl mercaptan   | 3.584  | 3.5     | ug/L  | 431602   | 1                     | 5.532  | 611133 | 5.0  |
| 1-Hexanol, 2-et... | 11.484 | 1.4     | ug/L  | 221642   | 3                     | 11.181 | 811131 | 5.0  |